ABSTRACTS

Second International Alloy Conference (IAC-2)
An Interdisciplinary Approach to the Science of Alloys in Metals, Minerals and Other Materials Systems

August 8-13, 1999
Davos, Switzerland

Conference Co-Chairs:
A. Gonis, A. Meike, K. Rajan and P.E.A. Turchi
Lawrence Livermore National Laboratory

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There will be no proceedings for this conference

14. ABSTRACT

This is a second Triennial Conference on the physical, chemical, and mechanical properties of materials, interpreted to mean simple and complex inorganic solids, i.e., metals, semiconductors, and mineral of technological and environmental significance

15. SUBJECT TERMS

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Session IA: *Thermodynamics of Alloys: Ordering*
Chairperson: A. Meike

E. K. H. Salje
Ordering mechanisms in minerals

H. Lang
Ordering kinetics in B_2-FeAl

V. Vaks
Kinetic features of non-simplest alloy orderings: DO_3, $L1_2$, and $L1_0$ type orderings

M. Spanl
Short-range ordering kinetics and microstructural development during post-deformation annealing

Session IA: *Thermodynamics of Alloys: Ordering*
Chairperson: K. Masuda-Jindo

F. Schmid
Order and disorder phenomena at surfaces of binary alloys

R. V. Chepulskyy
Analytical description of the short-range order in alloys with many-body atomic interactions

B. Wuensch
Changes in the atomic coordinates and state of anion and cation order induced by alloying in $Y_2[M(2)_Y M(1)_{1-Y}]_2 O_7$ solid solution systems

S. I. Simak
Ordering in Cu_2/NiZn: a first-principles Monte-Carlo study

FERROELASTICITY

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Abstract

The ferroelastic hysteresis is correlated with the propagation of twin walls under external stress. The wall thickness at T below Tc varies between 1nm and 7nm for different materials. Individual twin walls can act as fast diffusion paths for dopants and lattice imperfections. Several twin walls can combine to form hierarchical structures on a mesoscopic length scale (between, say 10nm and 100nm). Their features (needle domains, comb patterns, tweed and tartan patterns) are mainly determined by strain interactions with long correlation lengths. The formation of needle domains often leads to coarsening of the microstructure; their geometrical features are described in some detail.

ORDERING KINETICS IN B2-FeAl

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Chemistry

Changes in the degree of long-range order (LRO) have been investigated in B2-ordered
intermetallic Fe-44.8at%Al by residual resistometry. Order variations were observed during
isochronal and isothermal small step annealing after different thermal pre-treatment.
It is observed that atomic mobility in this alloy starts at about 500K. Between 500K and 700K
reversible changes of resistivity are interpreted as arising from local changes of order only.
Above 730K changes of LRO are observed which lead to the reversible adjustment of
equilibrium plateau values above 870K.
Two individual processes are found for both ordering regimes, which concern only local sample
areas and the total sample volume, respectively.

SHORT-RANGE ORDERING KINETICS AND MICROSTRUCTURAL DEVELOPMENT DURING POST-DEFORMATION ANNEALING

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During annealing after plastic deformation the initial degree of short-range order (SRO), the contribution of point defects to ordering kinetics and the development of SRO in the defected structure are changing simultaneously. In the present investigation the evolution of SRO during post-deformation annealing is compared for the three different binary alloys alpha-AuFe, alpha-AgZn, and alpha-CuAl.

Measurements of resistivity, differential scanning calorimetry (DSC) and microhardness were used to study SRO-kinetics in the presence of the changing defect structure during annealing. It was possible to separate resistivity changes caused by pure changes in SRO from resistivity changes being due to pure defect annealing by comparison with isothermal studies on the completely recrystallized alloys.

With a simple model for isothermal SRO-kinetics the data were fitted and vacancy parameters like formation and migration enthalpy as well as dislocation density were obtained.

ORDER AND DISORDER PHENOMENA AT SURFACES OF BINARY ALLOYS

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We present recent Monte Carlo results on surfaces of bcc-structured binary alloys which undergo an order-disorder phase transformation in the bulk. In particular, we discuss surface order and surface induced disorder at the bulk transition between the ordered (DO3) phase and the disordered (A2) phase. An intricate interplay between different ordering and segregation phenomena leads to a complex surface behavior, which depends on the orientation of the surface under consideration.

ANALYTICAL DESCRIPTION OF THE SHORT-RANGE IN ALLOYS WITH MANY-BODY ATOMIC INTERACTIONS

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The high-accuracy ring approximation elaborated in [1-3] by use of the thermodynamic fluctuation method in the context of the modified thermodynamic perturbation theory as applied to the lattice gas model is generalized for calculation of the short-range order parameters and their Fourier transform in disordered binary alloys with many-body atomic interactions of arbitrary order and effective radius of action. On the basis of the comparison with the Monte Carlo simulation data, the numerical accuracy of the derived approximation is studied. It is demonstrated that the temperature dependence of a position in reciprocal space of the short-range order Fourier transform's maximums is correctly described within this approximation.

[1] R.V. Chepulskii, J. Phys.: Condens. Matter (1998) 10 1505.

[2] R.V. Chepulskii and V.N. Bugaev, J. Phys.: Condens. Matter (1998) 10 7309; ibid. 7327.

[3] R.V. Chepulskii, J. Phys. Chem. Solids (1998) 59 1473.

CHANGES IN THE ATOMIC COORDINATES AND STATE OF ANION AND CATION ORDER INDUCED BY ALLOYING IN $Y_2[M(2)_YM(1)_{1-Y}]_2O_7$ SOLID SOLUTION SYSTEMS

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Many oxides with composition $A_2B_2O_7$, where A is a large trivalent cation and B a smaller quadrivalent species, assume the pyrochlore structure type, a superstructure of the cubic MO_2 fluorite structure with doubled lattice constant. The A3+ and B4+ ions order among M4+ sites in alternate 110 rows. Omission of one of eight oxygen ions in the fluorite array is necessary for charge balance. The arrangement of vacant sites is also ordered. The driving force for ordering was generally believed to be the size difference between the A3+ and B4+ ions.

We have synthesized several series of $Y_2(Zr,Sn,Ti)_2O_7$ pyrochlore solid solutions in which one species, M(1)4+, was progressively replaced by a larger M(2)4+ cation. Their structures were determined through Rietveld analysis of neutron powder diffraction data. The Zr_yTi_{1-y} and Zr_ySn_{1-y} series display very similar behavior. Increase in the fraction, y, of the larger species drives the system to a non-stoichiometric fluorite state with no long-range order when y exceeds 0.8. Remarkably, disorder in the anion and cation arrays proceed independently and at very different rates with increasing y. The vacant anion site fills linearly with y whereas the cations remain fully-ordered through much of the series and then display an abrupt transition to complete disorder that is reminiscent of Bragg-Williams-like behavior in a metallic alloy. Three distinct order parameters are necessary to describe the structures. The Sn_yTi_{1-y} system, in marked contrast to the preceding behaviors, remains fully ordered despite the fact that the range of radius ratios considerably overlaps that of the other systems. The state of order thus depends not only on differences in ionic size, but also on site preferences that we attribute to a covalent component to the bonding. A sharp rise in oxygen-ion conductivity (by 10^3) accompanies disorder in the anion array. The structural data provide satisfactory explanation of the variation of conductivity with y.

ORDERING IN CU₂NIZN: A FIRST-PRINCIPLES MONTE CARLO STUDY

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Monte Carlo simulations based on effective interactions obtained from $O(N)$ first-principles calculations reveal three order-disorder transitions in ternary Cu_2NiZn in contrast to the generally accepted picture which assumes the possibility for only *two*. We demonstrate that this sequence of transitions is a consequence of the symmetry of the ground state and the magnitude of the dominating pair interactions.

Session IB: *Thermodynamics of Alloys: Kinetics and diffusion*
Chairperson: G. Grimvall

W. E. Glassley
Using arrested solid-solid multiphase reactions in geological materials to deduce the rate of crystal uplift

M. Athenes
Kinetics of phase separation in a binary alloy: influence of the atomic mobilities

K. Rajan
Self Assembly in epitaxial semiconductor alloys

P. A. Khorzhavyi
***Ab initio* study of vacancies in metals and compounds**

W. Pfeiler
Point defect energies in $L1_2$-ordered Ni_3Al

USING ARRESTED SOLID - SOLID MULTIPHASE REACTIONS IN GEOLOGICAL MATERIALS TO DEDUCE THE RATE OF CRUSTAL UPLIFT

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The history geological terrains experience can be traced as a series of temperature and pressure changes. Each change drives the system toward a new state of thermodynamic equilibrium. The resultant overprinted rock fabrics, textures and chemical heterogeneities can be difficult to interpret. However, if carefully chosen, features from the scale of kilometers to nanometers can be used to reconstruct the history of mountain systems. Uplift of the Sri Lankan Central Highlands was rapid enough to preserve well-developed symplectite textures, some of which represent arrested solid-state diffusion-controlled reactions of garnet + O2 to form orthopyroxene + plagioclase + magnetite, as the rocks were exhumed from over 30 km in the earth's crust. Our objective has been to determine the reaction mechanisms responsible for symplectite development, and to establish the time interval over which these reactions occurred, to constrain the rate of mountain uplift. Considering that the most rapid mechanism is solid state grain-boundary diffusion of oxygen, the reaction time can be constrained by bounding the rate of oxygen supply to the reaction site. The solid state grain boundary diffusion rate of oxygen has been inferred to be ca. 10^{-14} m^2/sec (Farver and Yund, 1991), but is sensitive to inferred grain boundary width. The range of rates thus determined, allows the distinction between rapid uplift similar to that of the Himalayan Mountains, and the slow and progressive erosion of a less dramatic terrain. Further constraints on diffusion control and energetic relationships are determined from crystallographic relationships between the reactant and product phases, and submicron scale microstructures.

KINETICS OF PHASE SEPARATION IN A BINARY ALLOY:
BINARY ALLOY:
INFLUENCE OF THE ATOMIC MOBILITIES

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ABSTRACT

An atomistic kinetic model with a vacancy mediated diffusion mechanism is used to study the precipitation kinetics from a supersaturated solid solution. For a given equilibrium phase diagram, the asymmetry of the pairwise interaction energies determines the ratio of solute to solvent mobility.

We show that varying this energetical asymmetry, i.e. the vacancy-solute binding energy, affects the weight of the various n-mers contribution to the clustering process and modifies the phase separating kinetic pathway both for low and high solute supersaturation.

Moreover, we observe that decreasing the temperature increases the weight of the coagulation mechanism. This property of the vacancy dynamics explains why, in Fe-Cu system, precipitation kinetic measurements yield a Johnson-Mehl-Avrami exponent which increases with decreasing temperature. At variance, simulations using the direct exchange dynamics yield an exponent varying in the opposite direction.

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SELF-ASSEMBLY IN EPITAXIAL SEMICONDUCTOR ALLOYS

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With the development of new optoelectronic device architectures and applications there has been renewed and extensive interest in the fundamental issues governing phase stability in chemically complex epitaxial compound semiconductors. In this paper we review some of the recent experimental findings in this field and point out the importance of different microstructural length scales associated with the different types of phase instabilities associated with ternary and quaternary compounds. Of particular focus is the ability to take advantage of intrinsic thermodynamic and kinetic behavior of these complex semiconductor alloys in epitaxial structures to "engineer" compositional modulations of varying length scales which would not normally appear in bulk alloy systems. Hence new "self-assembled" microstructures can be generated. In this paper we outline the some of the crystallographic and structural characteristics of such self–assembled alloy systems and discuss the possible mechanisms governing their formation and stability.

AB INITIO STUDY OF VACANCIES IN METALS AND COMPOUNDS

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The results of *ab initio* calculations of the vacancy formation energies in all the transition and noble metals are presented. We also report on the formation and interaction energies of native point defects in the NiAl intermetallic compound. The calculations are performed within the locally self-consistent Green's function method and include multipole electrostatic corrections to the atomic sphere approximation. The results are in excellent agreement with experiment and existing full-potential calculations.

main topic area: 2
subtopic area: **b**

POINT DEFECT ENERGIES IN L1$_2$-ORDERED Ni$_3$Al.

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Experimental investigation of order-order relaxations in Ni$_3$Al by residual resistometry yielded a very high ordering activation energy of about 4.6eV being in correspondence with tracer experiments, where the tracer atom substitutes the Al-atom. Qualitatively, this might be interpreted by breaking of bonds to the 12 surrounding Ni nearest neighbour atoms of the ordered L1$_2$-lattice.

For the purpose of a more fundamental understanding the properties of vacancies and antisites in Ni$_3$Al were studied by means of *ab initio* calculations for supercells. Formation energies for Ni- and Al-vacancies were derived using a grandcanonical ensemble. Further, vacancy migration energies were determined successively displacing atoms from their equilibrium position to a vacant nearest neighbour position. Correlated jumps during a jump cycle were also taken into account.

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preferred: poster session

Session IC: *Thermodynamics of Alloys : phase stability and transformation*
Chairperson: W. E. Glassley

S. Saxena
Application of synchrotron light, CCD-devices and lasers to the study of materials

K. Masuda-Jindo
Effects of continuous atomic displacement on the phase stability of metallic alloys

G. Grimvall
Dynamical lattice instabilities in alloy phase diagrams

S. Fries
Computational thermodynamics: modelling and applications

T. Mohri
Susceptibility near the transition temperature calculated from first-principles

Chairperson: D. Papaconstantopoulos

W. Schweika
Diffuse scattering of Cu-Au alloys: displacements and Fermi-surface effects

V. Vinograd
Maximization of cluster entropy via an irreversible algorithm: application to the cluster variation method

C. Colinet
CVM calculations of the solid-state equilibria in the Fe-Co phase diagram

S. Shallcross
Onsager cavity field in statistical mechanics of alloys

APPLICATION OF SYNCHROTRON LIGHT, CCD-DEVICES AND LASERS TO THE STUDY OF MATERIALS

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The goal of the materials science is to understand the behavior of solids, melts and fluids over a range of pressures and temperatures, well enough to construct detailed, quantitative and predictive models of the physical and chemical processes operative in the industrial systems. In recent years, there have been significant technical improvements in generating and measuring high temperatures using lasers and spectroradiometry (multi wave-length pyrometry) and in-situ x-ray study of micrometer size heated samples using synchrotrons. These techniques permit us to extend the study of existing materials to higher temperatures and pressures more than ever before; they will also inevitably help us in conceiving and producing a whole range of new materials. Examples of some recent studies on iron, oxides and silicates will be presented.

Submitted to main topic area: 2. Thermodynamic properties

Subtopic area: a. Assessement of phase diagram, b. Ordering and phase tr..

EFFECTS OF CONTINUOUS ATOMIC DISPLACEMENT ON THE PHASE STABILITY OF METALLIC ALLOYS

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The continuous displacement (CD) formulation of the CVM allows atoms to be displaced from the reference rigid lattice points. When an atom displaced at r is regarded as a species r, the system is in an alloy of an infinite number of species and the CVM entropy can be applied to the system. The applications are presented for bcc and fcc binary alloys, within pair and quasi-chemical tetrahedron cluster approximations, respectively. For phase-separating binary alloys, the change of lattice constant with the composition and the reduction of the transition temperature are shown. For the order-disorder phase transition of bcc alloys, the transition temperatures are found to be reduced significantly compared to those of the conventional CVM. We also compare the calculation results with those derived by the moment method in the statistical mechanics.

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